THE DEVELOPMENT OF QUANTUM CHEMISTRY CODES

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The Cambridge Analytic Derivatives Package (CADPAC) has continued to be developed as a Computational Chemistry Package, in line with the grant proposal. During the period of this report the following extensions have been made.

(i) The calculation of the non-linear optical properties $\alpha(\omega;-\omega)$, $\beta(-\omega_1-\omega_2;\omega_1,\omega_2)$

(ii) The development of a high-spin open shell perturbation theory RMP2, ROMP2 code.

(iii) Brueckner theory at the Doubles and Triples level.

(iv) The Development of a Density Functional Code.

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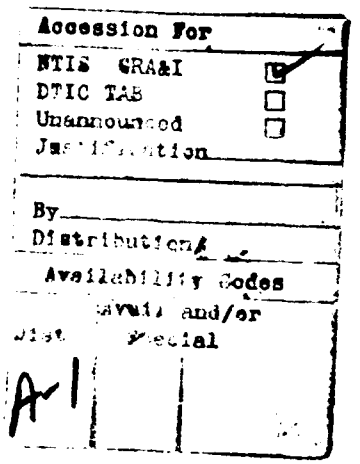
This report has been reviewed and is releasable to the National Technical Information Service (NTIS). At NTIS it will be releasable to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

OSAMA ELBAYOUMI, PhD
Chief, Chemistry

For DONALD R. ERBSCHLOE, Lt Col, USAF
Chief, International Programs



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Final Technical Report AFOSR-90-0225

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Full Period of Grant June 1 1990 - August 31 1993
Title of Grant " The Development of Quantum Chemistry Codes"

Over the entire period of the grant, we have continued to develop our Quantum Chemistry Code, CADPAC, as envisaged in the original grant application. Copies of CADPAC have been delivered to Wright Patterson AFB, Aberdeen Proving Grounds and Kirtland Supercomputer Institute (as well as many other U.S. centres not directly connected with USAF).

The specific advances which have been included in CADPAC in its latest version 5.2 are :

(i) Non linear Optical Properties : Frequency Dependent Self Consistent Field Polarisability $\alpha(-\omega;\omega)$ and Hyperpolarisability $\beta(-\omega_1-\omega_2;\omega_1,\omega_2)$. These important properties may now be calculated.

(ii) High-Spin Open Shell Perturbation Theory at second, third and fourth order (RMP2, 3, 4 and ROMP2, 3, 4). Gradients of RMP2 and ROMP2. The achievement here is that *Møller-Plesset theory is equally* applicable for open-shell as well as closed shell systems.

(iii) Brueckner theory has now been fully implemented at the BD(T) level, with analytic gradients, for closed shell systems. This version of Coupled Cluster Theory is gaining respectability.

(iv) Density Functional Theory. This has been an important development in Computational Chemistry recently. We have a high accuracy DFT code which solves the Kohn-Sham equations for the commonly used LDA and BLYP functionals. We have developed our own quadrature scheme, now widely used. We have available analytic gradients and second derivatives as well as electrical properties. We have developed our own functionals.

To achieve all the above highly successful developments has demanded considerable scientific manpower. We are grateful for the support of AFOSR at the level of one postdoctoral research assistant per annum. The personnel supported have been Drs. K. Laidig, C. W. Murray and A. Willetts.

Attached is a list of scientific papers which have been published in connection with these developments of CADPAC.

163. Frequency Dependent Hyperpolarizabilities with application to Formaldehyde and Methyl Fluoride. J E Rice, R D Amos, S M Colwell, N C Handy and J Sanz. J. Chem. Phys. 93, 8828 (1990).

169. Gradient Theory Applied to the Brueckner Doubles Method. R. Kobayashi, N.C. Handy, R.D. Amos, G.W. Trucks, M.J. Frisch and J.A. Pople. J. Chem. Phys. 95, 6723 (1991)

175. The Analytic Gradient of the Perturbative Triple Excitations Correction to the Brueckner Doubles Method. R. Kobayashi, R. D. Amos and N. C. Handy. Chem. Phys. Lett. 184, 195 (1991)

170. Bond Length and Reactivity: the Gauche Effect. A combined Crystallographic and Theoretical Investigation of the Effects of b-substituents on C-OX Bond Length. R.D. Amos, N.C. Handy, P.G. Jones, A.J.Kirby, J.K. Parker, J.M. Percy and M-D Su. J. Chem. Soc. Perkin Trans. 2, 549 (1992)

182. Comparison of the Brueckner and Coupled-Cluster Approaches to Electron Correlation. T. J. Lee, R. Kobayashi, N. C. Handy and R. D. Amos. J. Chem. Phys. 96, 8931 (1992)

187. Quadrature Schemes for Integrals of Density Functional Theory. C. W. Murray, N. C. Handy and G. J. Laming. Molec. Phys. 78, 997 (1993)

180. On the Optimisation of Exponents for *d* and *f* Polarisation Functions for First Row Atoms. M. J. Bearpark and N. C. Handy. Theor. Chim. Acta 84, 115 (1992)

193. Theory and Applications of Spin-Restricted Open-Shell Møller-Plesset Theory. D. J. Tozer, N. C. Handy, R. D. Amos, J. A. Pople, R. H. Nobes, X. Ming and H. F. Schaefer. Molec. Phys. 79, 777 (1993)

194. Electron Densities from the Brueckner Doubles method. C. M. van Heusden, R. Kobayashi, R. D. Amos and N. C. Handy. Theor. Chim. Acta 86, 25 (1993)

195. Kohn Sham Bond Lengths and Frequencies calculated with Accurate Quadrature and Large Basis Sets. C. W. Murray, G. J. Laming, N. C. Handy and R. D. Amos. Chem. Phys. Lett. 199, 551 (1992)

196 Gradient Theory Applied to Restricted (Open-Shell) Moller-Plesset Theory. D. J. Tozer, J. S. Andrews, R. D. Amos and N. C. Handy. Chem. Phys. Lett. 199, 229 (1992)

197. CADPAC5: The Cambridge Analytic Derivatives Package. R. D Amos, I. L. Alberts, J. S. Andrews, S. M. Colwell, N. C. Handy, D. Jayatilaka, P. J. Knowles, R. Kobayashi, N. Koga, K. E. Laidig, P. E. Maslen, C. W. Murray, J. E. Rice, J. Sanz, E. D. Simandiras, A. J. Stone and M.-D. Su. Cambridge (1992)

201. A Study of O_3, S_3, CH_2 and Be_2 using Kohn-Sham Theory with Accurate Quadrature and Large Basis Sets. C. W. Murray, N. C. Handy and R. D. Amos. J. Chem. Phys. 98, 7145 (1993)

213. Analytic Second Derivatives of the Potential Energy Surface. N. C. Handy, D. J. Tozer, G. J. Laming, C. W. Murray and R. D. Amos. Israel J. Chem. 33, 331 (1993)

214. The Determination of Hyperpolarisabilities using Density Functional Theory. S. M. Colwell, C. W. Murray, N. C. Handy and R. D. Amos. Chem. Phys. Lett. 210, 261 (1993)

216. A General Purpose Exchange-Correlation Energy Functional. G. J. Laming, V. Termath and N. C. Handy. J. Chem. Phys. 99, 8765 (1993)

218. Large Basis Set Calculations using Brueckner Theory. R. Kobayashi, R. D. Amos and N. C. Handy. J. Chem. Phys.